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16. ABSTRACT

Estimates from the model RAM were compared with actual SO_2 measurements from 13 Regional Air Pollution Study (RAPS) sites in St. Louis for 1976, with particular emphasis on the second highest concentrations for the 1-h, 3-h, and 24-h averaging times; the average annual concentration; and the top 5% of the distribution for the 24-h concentrations. Although there was considerable scatter in the comparison of the second highest concentrations, only 8 of the 39 data points were outside the bounds of a factor of two, and although there was more underestimation by the model as the averaging time increased, no overall bias was seen. Exponential distributions fit the top 5% of the 24-h concentration distributions for all sites for both the estimated and measured concentrations. The distributions for the estimated and measured concentrations matched at 8 of the 13 sites.

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COMPARISON OF RAM MODEL ESTIMATES WITH 1976 ST. LOUIS RAPS MEASUREMENTS OF SULFUR DIOXIDE

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Abstract—Comparisons of model estimates from the model RAM with SO_2 measurements from 13 Regional Air Pollution Study sites in St. Louis for the year 1976 were made with emphasis on 2nd highest concentrations for the 1-h, 3-h and 24-h averaging times, and also the top 5% of the distribution for 24-h concentrations. Although there is considerable scatter in the comparison of the 2nd highest concentrations, only 9 of 39 data points are outside the bounds of a factor of two and no overall bias is seen, although as the averaging time increases there is more underestimation by the model. Exponential distribution fit the top 5% of the 24-h concentration distributions for all stations for both estimated and measured concentrations. The distributions for estimated and measured concentrations were judged to match at eight of the thirteen sites.

Key word index: Urban dispersion model evaluations.

1. INTRODUCTION

Air quality simulation models have had increased use for projecting proposed source impact since the passage of the Clean Air Act Amendments in August 1977. Guidelines on air quality modeling have been issued by EPA (U. S. Environmental Protection Agency, 1978).

A knowledge of the accuracy of models is critical to their proper use in decision-making where comparison is made between estimated source impact with air quality standards. Available data bases should be used for model evaluation and results made available in order to accumulate a record of model performance.

This paper is directed to individuals concerned with the performance of Gaussian plume air-quality simulation models in estimating the high concentration values to be expected for 1, 3 and 24-h averaging times that occur once or twice a year. Such concentration values are often used in regulatory decision making. This paper contributes to the accumulation of knowledge on the performance of the model RAM (Novak and Turner, 1976; Turner and Novak, 1978a, 1978b) using detailed data from the Regional Air Pollution Study (RAPS) in St. Louis. This model has previously been evaluated using various data sets by Guldberg and Kern (1978), Kummler *et al.*, (1979), Ellis and Liu, (1981) and Hodanbosi and Peters (1981).

RAM is a steady-state model that uses the Gaussian model to calculate impact from point sources and calculates concentrations from area sources by numerical integration upwind from each receptor, as if from infinite crosswind line sources (employing the narrow plume hypothesis) with emissions determined according to the emission variation along the line upwind.

The calculated hourly concentrations from the model were previously made available to SRI International and were used for their evaluation (Ruff, 1981).

This data set was also used by Turner and Irwin (1983) to present data tables of highest, second-highest, fifth-highest and tenth-highest SO_2 concentrations observed and estimated for averaging times from 1-h to 1-y.

This paper summarizes those results with special attention being given to the results for the 3-h and the 24-h averaging times.

Ambient sulfur dioxide was routinely measured at 13 Regional Air Monitoring Stations (RAMS) in St. Louis as part of the Regional Air Pollution Study (RAPS). Seven of these sites are within 13 km of the center of St. Louis, five are at distances from 13 to 26 km and the other site is 50 km north. The locations of the RAMS sites and some of the major point sources are shown in Fig. 1. The number above the point source locations indicates the ranking of annual SO_2 emissions (1 = largest, 2 = second highest, etc.).

Emission inventories including SO_2 were compiled as part of RAPS such that hour-by-hour emissions can be calculated for the 196 point sources and 1989 area sources for the calendar year 1976. Area sources account for only 3.5% of the total annual emissions but are of considerable importance due to their low height of release above ground-level. Other investigations in St. Louis suggest that for some receptors, area sources contribute 50–60% to the total concentration. For the area sources, the annual average SO_2 emission rates ranged from 15.9×10^{-6} g ($m^2 s^{-1}$) to 1.0×10^{-9} g ($m^2 s^{-1}$), with 31% of the total area emissions accounted for by the 20×20 km area shown in

* On assignment from National Oceanic and Atmospheric Administration, United States Department of Commerce.

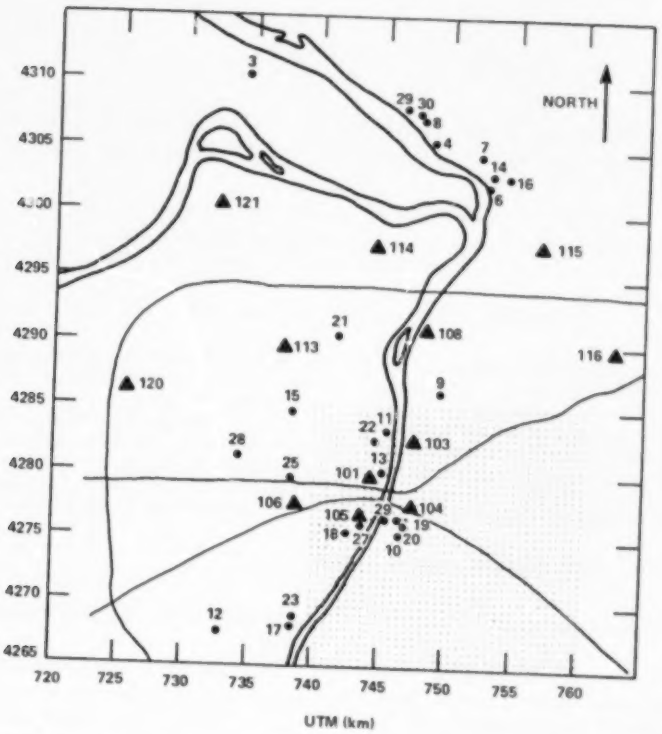

Fig. 1. Location of SO_2 monitoring sites and largest SO_2 point-source emitters in St. Louis. Numbers given above point-source locations indicate ranking (1, largest emission rate; 2, second largest emission rate, etc.) Solid triangles indicate monitoring sites. Solid circles indicate point-source locations. Values labeled along bottom and side of the figure are the UTM coordinates in kilometers. The 20 km square stippled indicates region containing major area-source emissions of SO_2.

Fig. 1. For the point sources, the annual average SO_2 emission rates ranged from 4294 $g\,s^{-1}$ to 0.01 $g\,s^{-1}$, with 90% of the emissions accounted for by 20 sources.

The RAM model was modified to accommodate the number of sources in the inventory and to use the emissions on the hourly basis. This model was executed for each hour of 1976 producing estimated hourly concentrations for each of the 13 receptors.

2. ANALYSIS

(a) *Annual and second-highest concentrations*

The comparison of estimated and measured annual concentrations and second-highest concentrations for three averaging times at each measurement station are summarized in Fig. 2. There is considerable scatter represented by the data for the 13 measurement locations but the mean bias shown in Table 1 for all four averaging periods are not significantly different from zero at the 95% confidence level. The standard deviation of residuals is a measure of the scatter and is given in Table 1. Note that compared to the mean measurement the standard deviation for the various averaging times ranges from about one-half to more than equal to the mean. Underestimation occurs more frequently (31 out of 52 for four averaging times) than overestimation. Factor of two lines are shown in Fig. 2. Of the 52 points in the figure, only eight are outside the factor of two bounds (three model overestimates and five underestimates).

The fractional error, $e = 2(E - M)/(E + M)$, where E is the model estimate and M is the measurement, can be used to examine model performance. The fractional error has the characteristic that it has the same numerical value but different signs for an overestimate of n times the measured value or an underestimate of $1/n$ times the measured value. Figure 3 displays a plot of the fractional errors for each station for the four averaging times considered. The fractional errors are arranged in order of magnitude so the values for individual stations are not identifiable except for station 104 which is identified by solid squares. These ordered fractional error curves allow determining the number of stations with estimates within any desired accuracy of the measurements. The bounds of a factor of 2 and a factor of 3 are shown in Fig. 3.

In using models to address regulatory matters,

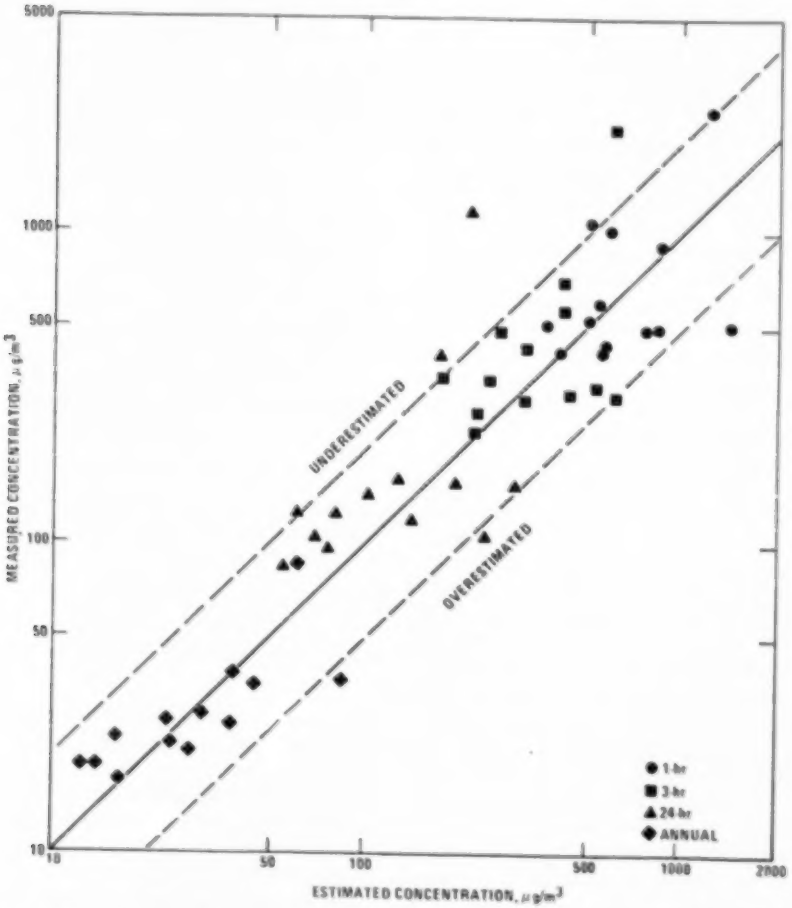

Fig. 2. Comparison of estimated and measured annual, second-highest 24-h, second-highest 3-h and second-highest 1-h SO_2 concentration at each monitoring site.

interest frequently centers on the highest value over the estimation network of the second-highest concentrations for each averaging-time of interest. These network second-highest maxima are shown in Fig. 4. Since there seemed to be some emissions inventory problems in the vicinity of measurement station 104 (measured concentrations increased quite significantly during the last two months of the year, see Ruff, 1981), network second-highest maxima are shown both for the entire network and for the network without station 104.

(b) *Exponential distribution from 20 highest concentrations*

Rao and Visalli (1981) found that an exponential function well approximated the cumulative frequency

Table 1. Statistics for annual and second-highest concentrations

	Mean residual* ($\mu g\ m^{-3}$)	Standard deviation of ($\mu g\ m^{-3}$)	Standard deviation over mean measurement	Mean fractional error
Annual	2.3	16.08	0.52	0.011
Second-highest 24-h	−88.0	269.5	1.18	−0.245
Second-highest 3-h	−146.1	433.5	0.84	−0.175
Second-highest 1-h	−47.6	494.6	0.65	0.016

* Residual is estimate minus measurement.

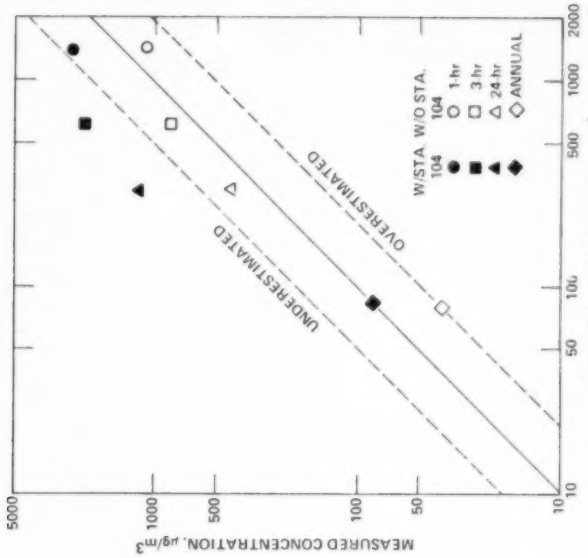

Fig. 4. Comparison of network maxima second highest SO_2 concentrations.

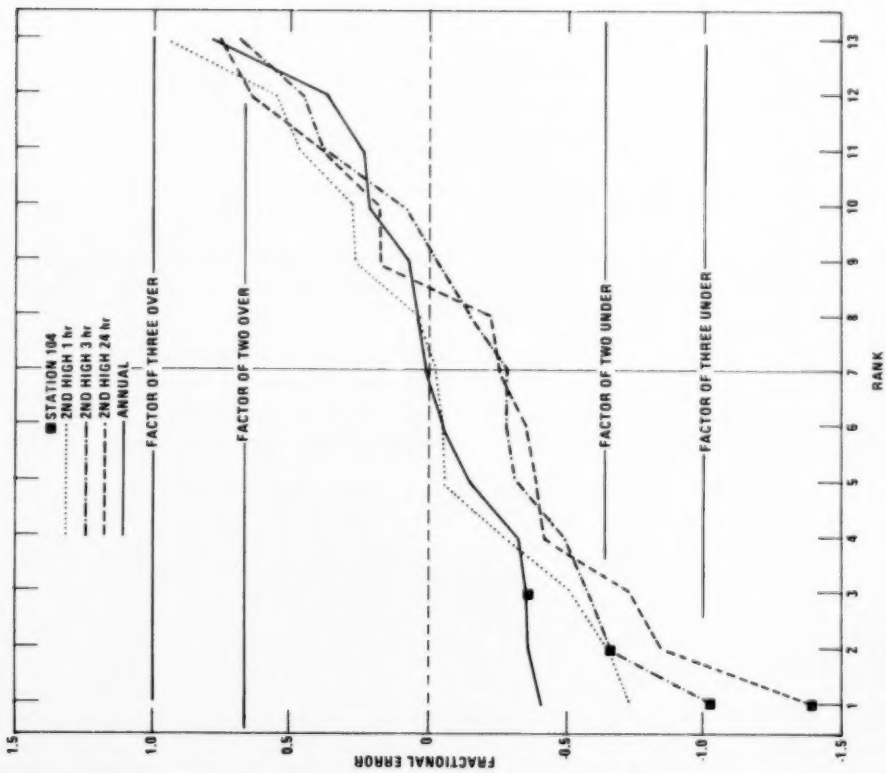

Fig. 3 Ordered fractional errors for annual and second-highest 24-h, 3-h and 1-h for the 13 monitoring sites.

function for the highest 5% of the concentration values. We chose to use the 20 highest concentration values as representative of the highest 5% of the data in order to simplify the analysis procedure. The cumulative frequencies for the censored data are computed according to the equation

$$\text{PROB}(\chi < x) = 1 - R/(n+1), \quad (1)$$

where PROB ($\chi < x$) = the probability that χ assumes any value less than x, n = the number of data values (20 in our case) used in the analysis and R = the rank order of the concentration value with 1 representing the highest value. The reasons for computing the cumulative frequencies with this equation are explained by Gumbel (1954) and Roberts (1979).

The assumed exponential cumulative frequency distribution function has the form

$$F\chi(x) = 1 - e^{-(x-A)/B} \quad \text{for} \quad x > A, \quad (2)$$

where the shape parameter B, and the location parameter A can be estimated using the maximum likehood methods as,

$$A = \min x_i \quad (3)$$

$$B = (1/n) \sum_i (x_i - \min x_i), \quad (4)$$

where the x_i's are concentration values in the upper percentile of interest. If the concentration values can be considered independent, continuous for $x > A$ and represent a variety of meteorological conditions, then the exact theory of extreme values can be employed to define the distribution functions for the highest and second-heighest values using the F_χ functions. These assumptions are most likely not met with these data, and hence we have not made direct use of extreme value theory. However, the results of fitting the cumulative frequency functions to the upper percentiles of the data do provide an alternate means for assessing model performance in estimating the highest concentration values. Table 2 summarizes the results of fitting the two-parameter exponential cumulative frequency functions to the highest 20 24-h average concentration values. The exponential distribution was fit to both the 24-h concentration values observed and to the values estimated by the RAM model. If an observed average concentration was available, that is, the 24-h period contained at least 22 h of observation, then the corresponding RAM model's estimate for the 24-h period was selected for use in the analysis. The Kolmogorov–Smirnov test was employed to test the goodness of fit of the two-parameter exponential cumulative frequency distributions to the data values. At the 0.05 level of significance, the hypothesis that the cumulative frequency distributions were of the form defined by (1) and (2), with the parameters given by (3) and (4), could not be rejected at any of the sites either for the measurements or for the RAM model estimates. The Kolmogorov–Smirnov test results may imply a better fit than actually is present if the concentration values are correlated. We can not dismiss this possibility.

For comparisons of the model estimates with the observed values for the upper 5% of the cumulative frequency function, all that is needed is a reasonably good description of the magnitude and variation of the values, which the two-parameter exponential function seems to supply. For both the location parameter A and the shape parameter B the ratio was formed of the parameter value from the estimates divided by the parameter value from the measurements. The parameter values were judged to be: similar for ratio values between 0.75 and 1.25, different for ratio values less than 0.50 or ratio values greater than 2.0, and

Table 2. Maximum likelihood estimates for the cumulative frequency function of the form $F_\chi(x) = 1 - e^{-(x-A)/B}$ for the highest 20 values of 24-h averaged SO_2 concentrations

	Measured concentrations			RAM modeled concentrations		
Site	A ($\mu g\,m^{-3}$)	B ($\mu g\,m^{-3}$)	Explained variance (r^2)	A ($\mu g\,m^{-3}$)	B ($\mu g\,m^{-3}$)	Explained variance (r^2)
101	82.7	25.5	0.98	176.7	42.0	0.99
103	60.0	27.0	0.84	73.7	20.2	0.97
104	394.8	228.2	0.99	125.9	22.8	0.97
105	78.7	28.8	0.94	101.3	31.1	1.00
106	88.3	62.4	0.91	80.9	29.7	0.99
108	68.0	18.2	0.99	64.3	20.5	0.95
113	70.0	21.0	0.99	54.0	12.7	0.95
114	63.1	30.2	0.98	49.3	16.0	0.99
115	53.1	18.5	1.00	69.5	44.0	0.96
116*	45.0	27.3	0.80	42.1	12.6	1.00
120	52.3	10.4	0.98	33.0	10.6	0.97
121	66.3	14.8	0.97	40.3	15.9	0.97
122	49.0	27.7	0.98	40.7	12.0	0.97

* The highest 24-h measured concentration was 3.12 times larger than the next highest 24-h concentration. Similar comparisons at the other sites yielded ratios ranging from 1.00 to 1.80. It is suspected that the highest value at 116 is in error. Recomputing without this high value yields 44.8 and 14.8 for A and B, respectively.

Table 3. Comparison of parameters from exponential distributions for estimated concentrations from the model with measured concentrations (station numbers are in the appropriate category)

		Location parameter, *A*			
		Similar	Somewhat similar	Different	Total
Shape Parameter, *B*	Similar	108 116*	105 120 121		5
	Somewhat similar	103 113 114		101	4
	Different	106 122	115	104	4
	Total	7	4	2	13

* Based on recomputed values or *A* and *B* as discussed in the footnote to Table 1.

somewhat different for values between 0.50 and 0.75 or between 1.25 and 2.0. The similarity of the parameters on the above basis is summarized in Table 3.

For the eight stations at which both the location parameter and the slope parameter were judged to be similar or somewhat similar, the estimates of the second-highest 24-h concentration values were all within $\pm 35\%$ of the measured values. Estimates of the second-highest concentration values at the other five stations were in error by more than a factor or two. The median value for B (estimated) divided by B (measured) was 0.85 and the median value for A (estimated) divided by A (measured) was 0.92.

These results suggest that the estimated cumulative frequency distributions of the highest 24-h values have flatter slopes in comparison to the measured distribution and a tendency to slightly underestimate the overall magnitude of the highest concentration values. The median value for the second-highest 24-h concentration estimated divided by the second-highest concentration measured was 0.70 with overestimates occurring at four of the thirteen stations. These comparison results of the second-highest concentration values are in accord with the conclusions reached based on a comparison of the slope and location parameters derived from the observed and estimated highest concentration values. Whether an exponential function is the best (or appropriate) characterization of the highest concentration values is beyond the scope of this analysis. But, we have determined that the exponential function is useful in summarizing the model's performance in estimating these concentration values.

3. CONCLUSIONS

Comparisons of modeled SO_2 concentrations with measured concentrations on the annual basis and for the second-highest values for three short-term averaging times indicate no significant model bias. Model estimates are for the most part within a factor of two of the measured concentration values.

The fit of an exponential function to the top twenty 24-h concentration for both estimated and observed values was not rejected by statistical test for any of the 13 monitoring locations. Comparison of the location and slope parameters for both estimated and observed 24-h concentration values suggest that the estimated cumulative frequency distributions tend to slightly underestimate the higher concentration values.

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